

Efficient PML for the wave equation

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Abstract. In the last decade, the perfectly matched layer (PML) approach has proved a flexible and accurate method for the simulation of waves in unbounded media. Most PML formulations, however, usually require wave equations stated in their standard second-order form to be reformulated as first-order systems, thereby introducing many additional unknowns. To circumvent this cumbersome and somewhat expensive step, we instead propose a simple PML formulation directly for the wave equation in its second-order form. Inside the absorbing layer, our formulation requires only two auxiliary variables in two space dimensions and four auxiliary variables in three space dimensions; hence it is cheap to implement. Since our formulation requires no higher derivatives, it is also easily coupled with standard finite difference or finite element methods. Strong stability is proved while numerical examples in two and three space dimensions illustrate the accuracy and long time stability of our PML formulation.

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1 Introduction

The accurate and reliable simulation of wave propagations in unbounded media is of fundamental importance in a wide range of applications. The perfectly matched layer (PML) approach [6] has proved a flexible and accurate method for the simulation of waves. It consists in surrounding the computational domain by an absorbing layer, which generates no reflections at its interface with the computational domain; hence, it is perfectly matched. Inside the absorbing layer a damping term is added to the wave equation, which acts only in the direction perpendicular to the layer. This approach is analogous to the physical treatment of the walls of an anechoic chamber and provides an alternative to absorbing or nonreflecting boundary conditions [11, 12, 14–16].

The initial PML formulation of Bérenger [6] was based on splitting the electromagnetic

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fields into two parts, the first containing the tangential derivatives and the second containing the normal derivatives; damping was then enforced only upon the normal component. Later Abarbanel and Gottlieb [1] showed that Bérenger's approach was only weakly well-posed due to the unphysical splitting of the field variables. Several strongly well-posed approaches have been suggested since, some of which were shown to be linearly equivalent [2, 20].

The PML approach has proved very successful in practice, because of its simplicity, versatility, and robust treatment of corners. Once discretized and truncated at a finite thickness, the layer is no longer perfectly absorbing and the optimal damping parameters need to be determined via numerical experiments. Stability properties of the PML approach has been analyzed in several works, such as in [1, 2, 7, 9] among others.

The best implementation in the time domain is still under debate. Most PML formulations require wave equations stated in their standard second-order form to be reformulated as first-order hyperbolic systems, thereby introducing many additional unknowns. Here we propose instead a simple PML formulation directly for the second-order wave equation both in two and in three space dimensions. Our formulation also requires fewer auxiliary variables than previous formulations for the second-order wave equation – see [3, 5, 19], for instance.

Our paper is organized as follows. In Section 2 we derive a PML formulation for the wave equation in its standard second-order form. By judiciously choosing the auxiliary variables in the Laplace transformed domain, the resulting PML modified equations require only two auxiliary variables in two dimensions and four auxiliary variables in three dimensions inside the absorbing layer. Next, in Section 3 we prove stability of our PML formulation by using standard theory from [18]. The finite difference discretization of the PML modified wave equation is shown in Section 4. In Section 5, our numerical results both in two and three space dimensions demonstrate the accuracy and long time stability of the PML formulation.

2 PML formulation

We consider a time dependent wave field u propagating through unbounded three dimensional space and assume that all sources and initial disturbances are confined to the rectangular domain $\Omega = [-a_1, a_1] \times [-a_2, a_2] \times [-a_3, a_3]$, $a_1, a_2, a_3 > 0$. Outside Ω , we further assume the speed of propagation $c > 0$ to be constant; hence, all waves are purely outgoing in the unbounded exterior $\mathbb{R}^3 \setminus \Omega$. Inside Ω , the wave field $u(x_1, x_2, x_3, t)$ satisfies

$$u_{tt} - \nabla \cdot (c^2 \nabla u) = f \quad t > 0, \quad (2.1)$$

$$u = u_0 \quad t = 0, \quad (2.2)$$

$$u_t = v_0 \quad t = 0. \quad (2.3)$$

We wish to truncate the unbounded exterior and thereby restrict the computation to the finite computational domain Ω . In doing so, we need to ensure that all waves propagat-

ing outward leave Ω without spurious reflection. Thus we shall surround Ω by a perfectly matched layer (PML) of thickness L_i , $i=1,2,3$, in each coordinate which is designed to absorb the waves exiting Ω . Inside the absorbing layer, u then satisfies a modified wave equation whose solutions decay exponentially fast with distance from the computational domain.

Following [1,2], we let \hat{u} denote the Laplace transform of u , defined as

$$\hat{u} = \hat{u}(\mathbf{x}, s) = \int_0^\infty e^{st} u(\mathbf{x}, t) dt, \quad s \in \mathbb{C}. \quad (2.4)$$

Outside Ω , \hat{u} then satisfies the Helmholtz equation,

$$s^2 \hat{u} = \frac{\partial}{\partial x_1} \left(c^2 \frac{\partial \hat{u}}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(c^2 \frac{\partial \hat{u}}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left(c^2 \frac{\partial \hat{u}}{\partial x_3} \right). \quad (2.5)$$

Next, we introduce the coordinate transformation

$$x_i \mapsto \tilde{x}_i := x_i + \frac{1}{s} \int_0^{x_i} \zeta_i(x) dx, \quad i=1,2,3, \quad (2.6)$$

where the damping profile ζ_i is positive inside the absorbing layer, $|x_i| > a_i$, $i=1,2,3$, but vanishes inside Ω . If we now require \hat{u} to satisfy the modified Helmholtz equation in those stretched coordinates,

$$s^2 \hat{u} = \frac{\partial}{\partial \tilde{x}_1} \left(c^2 \frac{\partial \hat{u}}{\partial \tilde{x}_1} \right) + \frac{\partial}{\partial \tilde{x}_2} \left(c^2 \frac{\partial \hat{u}}{\partial \tilde{x}_2} \right) + \frac{\partial}{\partial \tilde{x}_3} \left(c^2 \frac{\partial \hat{u}}{\partial \tilde{x}_3} \right), \quad (2.7)$$

it is well-known that u will remain unaltered inside Ω , but decay exponentially fast inside the layer; hence the absorbing layer will be perfectly matched. In fact, the (unsplit) PML modified Helmholtz equation (2.7) in the Laplace transformed domain is standard [1,2]. The difficulty lies in transforming (2.7) back to the time domain, without introducing high order derivatives or too many auxiliary variables.

From (2.6), we observe that partial differentiation with respect to \tilde{x}_i is related to partial differentiation with respect to the physical coordinate, x_i , through

$$\frac{\partial}{\partial \tilde{x}_i} = \frac{s}{s + \zeta_i} \frac{\partial}{\partial x_i}. \quad (2.8)$$

We now let $\gamma_i = \gamma_i(\zeta_i; s)$, $i=1,2,3$ denote

$$\gamma_i := 1 + \frac{\zeta_i}{s}. \quad (2.9)$$

Then, by replacing partial derivatives according to (2.8) and multiplying the resulting expression by $\gamma_1 \gamma_2 \gamma_3$, we rewrite (2.7) in physical coordinates as

$$s^2 \gamma_1 \gamma_2 \gamma_3 \hat{u} = \frac{\partial}{\partial x_1} \left(c^2 \frac{\gamma_2 \gamma_3}{\gamma_1} \frac{\partial \hat{u}}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(c^2 \frac{\gamma_3 \gamma_1}{\gamma_2} \frac{\partial \hat{u}}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left(c^2 \frac{\gamma_1 \gamma_2}{\gamma_3} \frac{\partial \hat{u}}{\partial x_3} \right). \quad (2.10)$$

From (2.9) we derive after some algebra the following identities:

$$\begin{aligned}\frac{\gamma_2 \gamma_3}{s \gamma_1} &= 1 + \frac{(\zeta_2 + \zeta_3 - \zeta_1)s + \zeta_2 \zeta_3}{(s + \zeta_1)s}, \\ \frac{\gamma_3 \gamma_1}{s \gamma_2} &= 1 + \frac{(\zeta_3 + \zeta_1 - \zeta_2)s + \zeta_3 \zeta_1}{(s + \zeta_2)s}, \\ \frac{\gamma_1 \gamma_2}{s \gamma_3} &= 1 + \frac{(\zeta_1 + \zeta_2 - \zeta_3)s + \zeta_1 \zeta_2}{(s + \zeta_3)s}.\end{aligned}\tag{2.11}$$

By using (2.11) in (2.10) we find

$$\begin{aligned}& \left(s^2 + s(\zeta_1 + \zeta_2 + \zeta_3) + (\zeta_1 \zeta_2 + \zeta_2 \zeta_3 + \zeta_3 \zeta_1) + \frac{\zeta_1 \zeta_2 \zeta_3}{s} \right) \hat{u} \\ &= \frac{\partial}{\partial x_1} \left(c^2 \frac{\partial \hat{u}}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(c^2 \frac{\partial \hat{u}}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left(c^2 \frac{\partial \hat{u}}{\partial x_3} \right) \\ &+ \frac{\partial}{\partial x_1} \left(c^2 \left(\frac{(\zeta_2 + \zeta_3 - \zeta_1)s + \zeta_2 \zeta_3}{(s + \zeta_1)s} \right) \frac{\partial \hat{u}}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(c^2 \left(\frac{(\zeta_3 + \zeta_1 - \zeta_2)s + \zeta_3 \zeta_1}{(s + \zeta_2)s} \right) \frac{\partial \hat{u}}{\partial x_2} \right) \\ &+ \frac{\partial}{\partial x_3} \left(c^2 \left(\frac{(\zeta_1 + \zeta_2 - \zeta_3)s + \zeta_1 \zeta_2}{(s + \zeta_3)s} \right) \frac{\partial \hat{u}}{\partial x_3} \right).\end{aligned}\tag{2.12}$$

Next, we introduce the auxiliary functions ψ and $\boldsymbol{\phi} = (\phi_1, \phi_2, \phi_3)^\top$,

$$\begin{aligned}\hat{\psi} &= \frac{1}{s} \hat{u}, \\ \hat{\phi}_1 &= c^2 \left(\frac{\zeta_2 + \zeta_3 - \zeta_1}{s + \zeta_1} + \frac{\zeta_2 \zeta_3}{(s + \zeta_1)s} \right) \frac{\partial \hat{u}}{\partial x_1}, \\ \hat{\phi}_2 &= c^2 \left(\frac{\zeta_3 + \zeta_1 - \zeta_2}{s + \zeta_2} + \frac{\zeta_3 \zeta_1}{(s + \zeta_2)s} \right) \frac{\partial \hat{u}}{\partial x_2}, \\ \hat{\phi}_3 &= c^2 \left(\frac{\zeta_1 + \zeta_2 - \zeta_3}{s + \zeta_3} + \frac{\zeta_1 \zeta_2}{(s + \zeta_3)s} \right) \frac{\partial \hat{u}}{\partial x_3},\end{aligned}$$

or equivalently

$$\begin{aligned}s \hat{\psi} &= \hat{u}, \\ (s + \zeta_1) \hat{\phi}_1 &= c^2 \left((\zeta_2 + \zeta_3 - \zeta_1) + \frac{\zeta_2 \zeta_3}{s} \right) \frac{\partial \hat{u}}{\partial x_1}, \\ (s + \zeta_2) \hat{\phi}_2 &= c^2 \left((\zeta_3 + \zeta_1 - \zeta_2) + \frac{\zeta_3 \zeta_1}{s} \right) \frac{\partial \hat{u}}{\partial x_2}, \\ \text{and } (s + \zeta_3) \hat{\phi}_3 &= c^2 \left((\zeta_1 + \zeta_2 - \zeta_3) + \frac{\zeta_1 \zeta_2}{s} \right) \frac{\partial \hat{u}}{\partial x_3}.\end{aligned}$$

Finally, we use the above relations in (2.12) and transform the resulting equations back to the time domain, which yields the PML modified wave equation

$$\begin{aligned} u_{tt} + (\zeta_1 + \zeta_2 + \zeta_3)u_t + (\zeta_1\zeta_2 + \zeta_2\zeta_3 + \zeta_3\zeta_1)u &= \nabla \cdot (c^2 \nabla u) + \nabla \cdot \boldsymbol{\phi} - \zeta_1\zeta_2\zeta_3\psi, \\ \boldsymbol{\phi}_t &= \Gamma_1 \boldsymbol{\phi} + c^2 \Gamma_2 \nabla u + c^2 \Gamma_3 \nabla \psi, \\ \psi_t &= u, \end{aligned} \quad (2.13)$$

where

$$\begin{aligned} \Gamma_1 &= \begin{bmatrix} -\zeta_1 & 0 & 0 \\ 0 & -\zeta_2 & 0 \\ 0 & 0 & -\zeta_3 \end{bmatrix}, \quad \Gamma_2 = \begin{bmatrix} \zeta_2 + \zeta_3 - \zeta_1 & 0 & 0 \\ 0 & \zeta_3 + \zeta_1 - \zeta_2 & 0 \\ 0 & 0 & \zeta_1 + \zeta_2 - \zeta_3 \end{bmatrix} \\ \text{and } \Gamma_3 &= \begin{bmatrix} \zeta_2\zeta_3 & 0 & 0 \\ 0 & \zeta_3\zeta_1 & 0 \\ 0 & 0 & \zeta_1\zeta_2 \end{bmatrix}. \end{aligned}$$

In the interior of Ω , the damping profiles $\zeta_i, i=1,2,3$ and the auxiliary variables $\boldsymbol{\phi}, \psi$ vanish; hence, (2.13) reduces to (2.1) in Ω . Because our PML formulation (2.13) requires only four auxiliary scalar variables $\phi_1, \phi_2, \phi_3, \psi$ inside the layer and no high order derivatives, its implementation is not only straightforward but also cheap to implement.

In two space dimensions, ζ_3 and ϕ_3 and ψ vanish and our PML formulation reduces to

$$\begin{aligned} u_{tt} + (\zeta_1 + \zeta_2)u_t + \zeta_1\zeta_2u &= \nabla \cdot (c^2 \nabla u) + \nabla \cdot \boldsymbol{\phi}, \\ \boldsymbol{\phi}_t &= \Gamma_1 \boldsymbol{\phi} + c^2 \Gamma_2 \nabla u, \end{aligned} \quad (2.14)$$

where

$$\Gamma_1 = \begin{bmatrix} -\zeta_1 & 0 \\ 0 & -\zeta_2 \end{bmatrix}, \quad \Gamma_2 = \begin{bmatrix} \zeta_2 - \zeta_1 & 0 \\ 0 & \zeta_1 - \zeta_2 \end{bmatrix}.$$

Remarkably only two auxiliary functions are needed here.

The choice of the damping profiles $\zeta_i(x) \geq 0, i=1,2,3$ is arbitrary; it can be constant, linear, or quadratic among others. In our computations, we always use

$$\zeta_i(x_i) = \begin{cases} 0 & \text{for } |x_i| < a_i, \quad i=1,2,3 \\ \bar{\zeta}_i \left(\frac{|x_i - a_i|}{L_i} - \frac{\sin\left(\frac{2\pi|x_i - a_i|}{L_i}\right)}{2\pi} \right) & \text{for } a_i \leq |x_i| \leq a_i + L_i, \quad i=1,2,3. \end{cases} \quad (2.15)$$

Because $\zeta_i(x)$ is twice continuously differentiable throughout the interface at $|x_i| = a_i$, no special transmission conditions are needed there. The constant $\bar{\zeta}_i$ depends on the discretization and the thickness of the layer, which in practice is truncated by a homogeneous Dirichlet (or Neumann) boundary condition. Then the relative reflection, R , is given by

$$\bar{\zeta}_i = \frac{c}{L_i} \log\left(\frac{1}{R}\right), \quad i=1,2,3. \quad (2.16)$$

In Figure 1 we show damping profiles for different values of $\bar{\zeta}_i$.

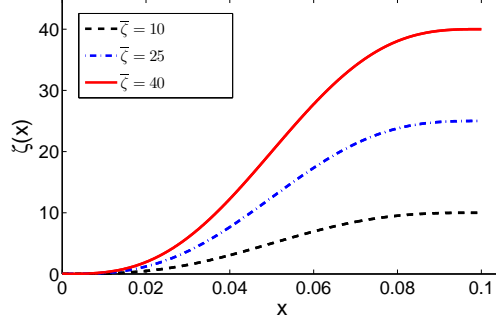


Figure 1: The damping profile $\zeta_i(x_i)$ given by (2.15) is shown for different values of $\bar{\zeta}_i$, with $c=1$ and $L_i=0.1$.

3 Stability

We now establish the stability and well-posedness of our PML formulation, first in two and then in three space dimensions, where we assume that the absorbing layer extends to infinity. Here we follow standard stability theory for hyperbolic systems [18], which we briefly recall below.

Consider a general Cauchy problem,

$$U_t = P\left(\frac{\partial}{\partial x}\right)U, \quad 0 \leq t \leq T, \quad U \in \mathbb{R}^p, \quad (3.1)$$

where $P(\partial_x)$ denotes a linear differential operator, with initial conditions

$$U(x,0) = U_0(x), \quad x \in \mathbb{R}^3. \quad (3.2)$$

Following [18], the Cauchy Problem is *weakly (resp. strongly) well-posed*, if the solution $U(\cdot, t)$ satisfies

$$\|U(\cdot, t)\|_{L_2} \leq K e^{at} \|U(\cdot, 0)\|_{H^s} \quad (3.3)$$

with $s > 0$ (resp. $s = 0$). The Cauchy Problem is *weakly (resp. strongly) stable*, if the solution $U(\cdot, t)$ satisfies

$$\|U(\cdot, t)\|_{L_2} \leq K(1+t)^s \|U(\cdot, 0)\|_{H^s} \quad (3.4)$$

with $s > 0$ (resp. $s = 0$). A necessary and sufficient condition for weak *well-posedness (resp. stability)* is that all eigenvalues λ of the operator $P(ik)$ satisfy

$$\Re\{\lambda(P(ik))\} \leq C, \quad k \in \mathbb{R}, \quad (3.5)$$

with $C > 0$ (resp. $C = 0$) independent of k . For strong *well-posedness (resp. stability)*, the corresponding eigenvectors must also be complete.

By rewriting the PML-modified wave equations (2.13), (2.14) as a first-order hyperbolic system and applying the stability theory from [18] delineated above, we can prove the following two stability results.

Theorem 3.1. The Cauchy problem for the PML formulation (2.14) in two space dimensions is strongly stable for $\zeta_1, \zeta_2 \geq 0$.

proof)

For simplicity, we assume that ζ_1, ζ_2 are constant; note, however, that the stability theory from [18] extends to smoothly varying coefficients. We introduce the new variable \mathbf{v} to rewrite the first equation in (2.14) equivalently as

$$u_t = -\zeta_2 u + \operatorname{div} \mathbf{v}, \quad \mathbf{v}_t = -\zeta_1 \mathbf{v} + c^2 \nabla u + \boldsymbol{\phi}. \quad (3.6)$$

By using (3.6), we now rewrite (2.14) as a first order hyperbolic system:

$$U_t = AU_x + BU_y + C, \quad (3.7)$$

where

$$U_t = (u, \phi_1, \phi_2, \mathbf{v}_1, \mathbf{v}_2)^\top, \quad (3.8)$$

$$A = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ c^2(\zeta_2 - \zeta_1) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ c^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ c^2(\zeta_1 - \zeta_2) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ c^2 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad (3.9)$$

$$\text{and } C = - \begin{bmatrix} \zeta_2 & 0 & 0 & 0 & 0 \\ 0 & \zeta_1 & 0 & 0 & 0 \\ 0 & 0 & \zeta_2 & 0 & 0 \\ 0 & 0 & 0 & \zeta_1 & 0 \\ 0 & 0 & 0 & 0 & \zeta_1 \end{bmatrix}.$$

By using a symbolic algebra program we find that the eigenvalues of the principal part of $P(ik)$ for (3.7) are

$$\lambda(P(ik)) = \pm ic(k_1^2 + k_2^2)^{1/2}. \quad (3.10)$$

Thus,

$$\Re\{\lambda(P(ik))\} = 0, \quad (3.11)$$

while the corresponding eigenvectors are also complete for all $\zeta_1, \zeta_2 \geq 0$. Therefore, since C is a diagonal matrix with negative entries for $\zeta_1, \zeta_2 \geq 0$, we conclude that (2.14) is strongly stable.

Theorem 3.2. The Cauchy problem for the PML formulation (2.13) in three space dimensions is strongly stable, if at least two $\zeta_j = 0, j = 1, 2, 3$, and weakly stable, otherwise.

proof)

We introduce the new variable \mathbf{v} to rewrite the first equation in (2.13) as

$$u_t = -\zeta_2 u + \operatorname{div} \mathbf{v} - \zeta_3 \psi, \quad \mathbf{v}_t = -\zeta_1 \mathbf{v} + c^2 \nabla u + \boldsymbol{\phi}. \quad (3.12)$$

By using (3.12), we can rewrite (2.13) as a first order hyperbolic system:

$$U_t = AU_x + BU_y + CU_z + D, \quad (3.13)$$

where

$$U_t = (u, \phi_1, \phi_2, \phi_3, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \psi)^\top, \quad (3.14)$$

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ c^2(\zeta_2 + \zeta_3 - \zeta_1) & 0 & 0 & 0 & 0 & 0 & 0 & \zeta_2\zeta_3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad (3.15)$$

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c^2(\zeta_3 + \zeta_1 - \zeta_2) & 0 & 0 & 0 & 0 & 0 & 0 & \zeta_3\zeta_1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad (3.16)$$

and

$$C = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c^2(\zeta_1 + \zeta_2 - \zeta_3) & 0 & 0 & 0 & 0 & 0 & 0 & \zeta_1\zeta_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \quad (3.17)$$

By using a symbolic algebra program, we find that the eigenvalues λ of $P(ik)$ for (3.13) are

$$\lambda(P(ik)) = \pm ic(k_1^2 + k_2^2 + k_3^2)^{1/2}. \quad (3.18)$$

Thus,

$$\Re\{\lambda(P(ik))\} = 0, \quad (3.19)$$

while the corresponding eigenvectors are also complete, if at least two $\zeta_j = 0, j = 1, 2, 3$; else, they are not complete. Therefore, since D is a diagonal matrix with negative entries for $\zeta_1, \zeta_2, \zeta_3 \geq 0$, we conclude that (2.13) is strongly stable, if at least two $\zeta_j = 0$, and weakly stable, otherwise.

4 Finite difference discretization

Here we show how to discretize (2.13) with standard second-order finite differences on a uniform mesh at grid points $x_{i,i_\ell} = x_{1,0} + i_\ell \Delta x_i$, with $i=1,2,3$ and $i_\ell=0,1,\dots,M_\ell$. For the time discretization we use a constant step size Δt and denote the time levels by $t_n = t_0 + n\Delta t$, $n=0,1,\dots,N$. Inside the absorbing layer, we further introduce a space-time staggered grid at locations $x_{i,i_\ell+\frac{1}{2}} = x_{i,0} + (i_\ell + \frac{1}{2}) \Delta x_i$, $i=1,2,3$ and times $t_{n+\frac{1}{2}} = t_0 + (n + \frac{1}{2}) \Delta t$. Then the numerical solution $u_{i,j,k}^n$, which approximates u at grid point $(x_{1,i}, x_{2,j}, x_{3,k})$ and time t_n , satisfies

$$\begin{aligned} & \frac{u_{i,j,k}^{n+1} - 2u_{i,j,k}^n + u_{i,j,k}^{n-1}}{\Delta t^2} + (\zeta_{1i} + \zeta_{2j} + \zeta_{3k}) \frac{u_{i,j,k}^{n+1} - u_{i,j,k}^{n-1}}{2\Delta t} + (\zeta_{1i}\zeta_{2j} + \zeta_{2j}\zeta_{3k} + \zeta_{3k}\zeta_{1i}) u_{i,j,k}^n \\ = & \frac{c_{i+\frac{1}{2},j,k}^2 u_{i+1,j,k}^n - (c_{i+\frac{1}{2},j,k}^2 + c_{i-\frac{1}{2},j,k}^2) u_{i,j,k}^n + c_{i-\frac{1}{2},j,k}^2 u_{i-1,j,k}^n}{\Delta x_1^2} \\ & + \frac{c_{i,j+\frac{1}{2},k}^2 u_{i,j+1,k}^n - (c_{i,j+\frac{1}{2},k}^2 + c_{i,j-\frac{1}{2},k}^2) u_{i,j,k}^n + c_{i,j-\frac{1}{2},k}^2 u_{i,j-1,k}^n}{\Delta x_2^2} \\ & + \frac{c_{i,j,k+\frac{1}{2}}^2 u_{i,j,k+1}^n - (c_{i,j,k+\frac{1}{2}}^2 + c_{i,j,k-\frac{1}{2}}^2) u_{i,j,k}^n + c_{i,j,k-\frac{1}{2}}^2 u_{i,j,k-1}^n}{\Delta x_3^2} \\ & + \frac{\tilde{\phi}_{1i+\frac{1}{2},j,k}^n - \tilde{\phi}_{1i-\frac{1}{2},j,k}^n}{\Delta x_1} + \frac{\tilde{\phi}_{2i,j+\frac{1}{2},k}^n - \tilde{\phi}_{2i,j-\frac{1}{2},k}^n}{\Delta x_2} + \frac{\tilde{\phi}_{3i,j,k+\frac{1}{2}}^n - \tilde{\phi}_{3i,j,k-\frac{1}{2}}^n}{\Delta x_3} - \zeta_{1i} \zeta_{2j} \zeta_{3k} \frac{\psi_{i,j,k}^{n+\frac{1}{2}} + \psi_{i,j,k}^{n-\frac{1}{2}}}{2}, \end{aligned}$$

where the cell averages of the auxiliary functions ϕ_1 , ϕ_2 and ϕ_3 are defined as

$$\begin{aligned} \tilde{\phi}_{1i+\frac{1}{2},j,k}^n &= \frac{1}{4} \left(\phi_{1i+\frac{1}{2},j-\frac{1}{2},k-\frac{1}{2}}^n + \phi_{1i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}^n + \phi_{1i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}^n + \phi_{1i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^n \right), \\ \tilde{\phi}_{2i,j+\frac{1}{2},k}^n &= \frac{1}{4} \left(\phi_{2i-\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}^n + \phi_{2i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^n + \phi_{2i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}^n + \phi_{2i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^n \right), \\ \tilde{\phi}_{3i,j,k+\frac{1}{2}}^n &= \frac{1}{4} \left(\phi_{3i-\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}^n + \phi_{3i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^n + \phi_{3i+\frac{1}{2},j-\frac{1}{2},k+\frac{1}{2}}^n + \phi_{3i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^n \right). \end{aligned}$$

Concurrently with the above discretized wave equation, we also advance the (scalar) auxiliary variables ψ , ϕ_j , $j=1,2,3$ inside the absorbing layer by using standard finite differences. For ψ we use

$$\frac{\psi_{i,j,k}^{n+\frac{1}{2}} - \psi_{i,j,k}^{n-\frac{1}{2}}}{\Delta t} = u_{i,j,k}^n$$

whereas for ϕ_1 we use

$$\begin{aligned} & \frac{\phi_{1+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+1} - \phi_{1+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^n}{\Delta t} \\ &= -\zeta_{1+\frac{1}{2}} \frac{\phi_{1+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+1} + \phi_{1+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^n}{2} + \left(\zeta_{2j+\frac{1}{2}} + \zeta_{3k+\frac{1}{2}} - \zeta_{1+\frac{1}{2}} \right) D_{x_1}^h u_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} \\ & \quad + \zeta_{2j+\frac{1}{2}} \zeta_{3k+\frac{1}{2}} D_{x_1}^h \psi_{1+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}}, \end{aligned}$$

where

$$\begin{aligned} D_{x_1}^h u_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{2} \left(\frac{\tilde{u}_{i+1,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} - \tilde{u}_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1}}{\Delta x_1} + \frac{\tilde{u}_{i+1,j+\frac{1}{2},k+\frac{1}{2}}^n - \tilde{u}_{i,j+\frac{1}{2},k+\frac{1}{2}}^n}{\Delta x_1} \right), \\ D_{x_1}^h \psi_{1+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{\tilde{\psi}_{i+1,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - \tilde{\psi}_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x_1}. \end{aligned}$$

Here, the cell averages of u and ψ are defined as

$$\begin{aligned} \tilde{u}_{i,j+\frac{1}{2},k+\frac{1}{2}}^n &= \frac{1}{4} \left(u_{i,j,k}^n + u_{i,j,k+1}^n + u_{i,j+1,k}^n + u_{i,j+1,k+1}^n \right), \\ \tilde{\psi}_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4} \left(\psi_{i,j,k}^{n+\frac{1}{2}} + \psi_{i,j,k+1}^{n+\frac{1}{2}} + \psi_{i,j+1,k}^{n+\frac{1}{2}} + \psi_{i,j+1,k+1}^{n+\frac{1}{2}} \right). \end{aligned}$$

The finite difference approximations for ϕ_2 and ϕ_3 are analogous.

5 Numerical experiments

Here we present numerical experiments that illustrate the accuracy, versatility and long-time stability of our PML formulation discretized with standard finite differences as in Section 4. In all cases we choose $\tilde{\zeta}_i = 80$ in the damping profile, which yields a relative reflection $R \approx 10^{-3}$ for the typical values $c = 1$ and $L_i = 0.1$. At the exterior boundary of the absorbing layer we impose homogeneous Dirichlet boundary conditions.

5.1 Point source in 2D

First, we consider the wave equation (2.1) in two space dimensions with constant speed of propagation $c=1$ and zero initial conditions, $u_0=v_0=0$. The source term f corresponds to a truncated first derivative of a Gaussian:

$$f(x,y,t) = \delta(x) \delta(y) h(t) \quad (5.1)$$

with

$$h(t) = \frac{d}{dt} (e^{-\pi^2 (f_0 t - 1)^2}), \quad f_0 = 10 \text{ Hz}. \quad (5.2)$$

The grid spacing is uniform in x_1 and x_2 , with $\Delta x = 0.002$.

In Figure 2 we display snapshots of the numerical solutions at different times in $\Omega = [-0.5, 0.5]^2$, surrounded by a PML of width $L = 0.1$. We observe how the circular wave propagates outward essentially without spurious reflection from the PML. By time $t = 1$ the wave has essentially left the computational domain. To assess the error in the numerical solution, we compute a reference solution in a much larger domain of size $[-5.5, 5.5] \times [5.5, 5.5]$, so that boundary effects are postponed to later times inside Ω . In Figure 3, the time evolution of the L^2 -error is shown for different values of the damping coefficient $\bar{\zeta}_i$. Until $t = 8$ we observe a steady decrease of the error over seven orders of magnitude, regardless of the value of $\bar{\zeta}_i$, which demonstrates the long-time stability of our method. Moreover, our formulation appears robust with respect to the parameter value $\bar{\zeta}_i$.

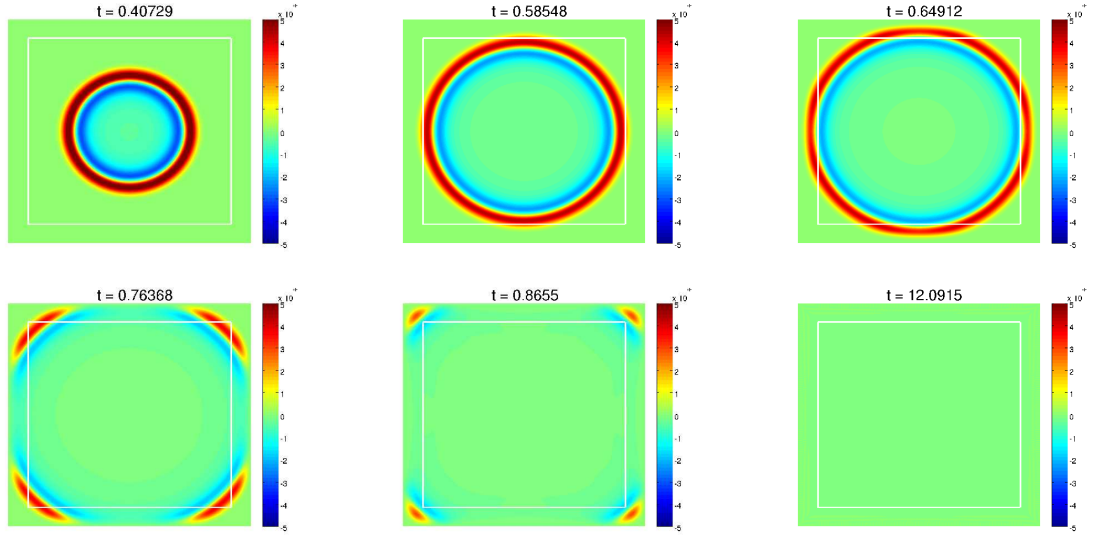


Figure 2: Point source in 2D: snapshots of the numerical solutions at different times in $\Omega = [-0.5, 0.5]^2$, surrounded by a PML of width $L = 0.1$.

5.2 Heterogeneous medium in 2D

Next, to illustrate the versatility of our PML formulation, we consider the homogeneous wave equation (2.1) in a heterogeneous medium with varying wave speed $c = c(x_2)$, given

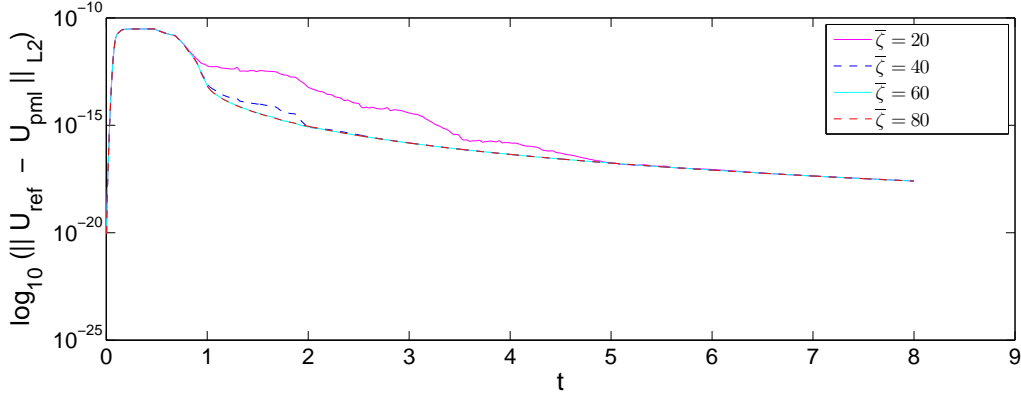


Figure 3: Point source in 2D: time evolution of the L_2 -error for different damping coefficients $\bar{\zeta}_i$.

by

$$c(x_1, x_2) = \begin{cases} 0.5, & \text{if } x_2 < -b \\ 1 + \frac{y}{2b} + \frac{1}{2\pi} \sin\left(\frac{\pi x_2}{b}\right), & \text{if } |x_2| < b \\ 1.5, & \text{otherwise.} \end{cases} \quad (5.3)$$

We set $b = 0.95$ which yields the vertical velocity profile shown in Figure 4. The initial conditions are

$$u|_{t=0} = u_0(x_1, x_2) \quad \text{and} \quad u_t|_{t=0} = 0, \quad (5.4)$$

where

$$u_0(x_1, x_2) = \begin{cases} (4(x_1 + 0.4)(0.4 - x_1))^3 \sin(3\pi x_2), & \text{if } -0.4 < x_1 < 0.4, -1 < x_2 < 1 \\ 0, & \text{otherwise.} \end{cases}$$

Here Ω is the square domain $[-1, 1] \times [-1, 1]$, surrounded by a PML of width $L = 0.2$. The

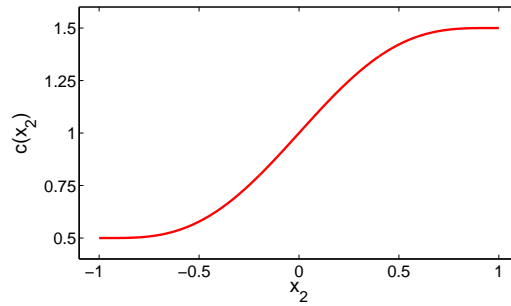


Figure 4: Heterogeneous medium in 2D: varying wave speed c given by (5.3).

finite difference grid is uniform with grid spacing $\Delta x = 0.004$. In Fig.5, we display snapshots of the solution at different times, where again the last frame is purposely chosen at a much later time. In spite of the varying wave speed and the glancing angle of incidence along the vertical artificial boundaries, the waves are damped without spurious reflection. Even at much later times we do not observe any instability in the numerical scheme.

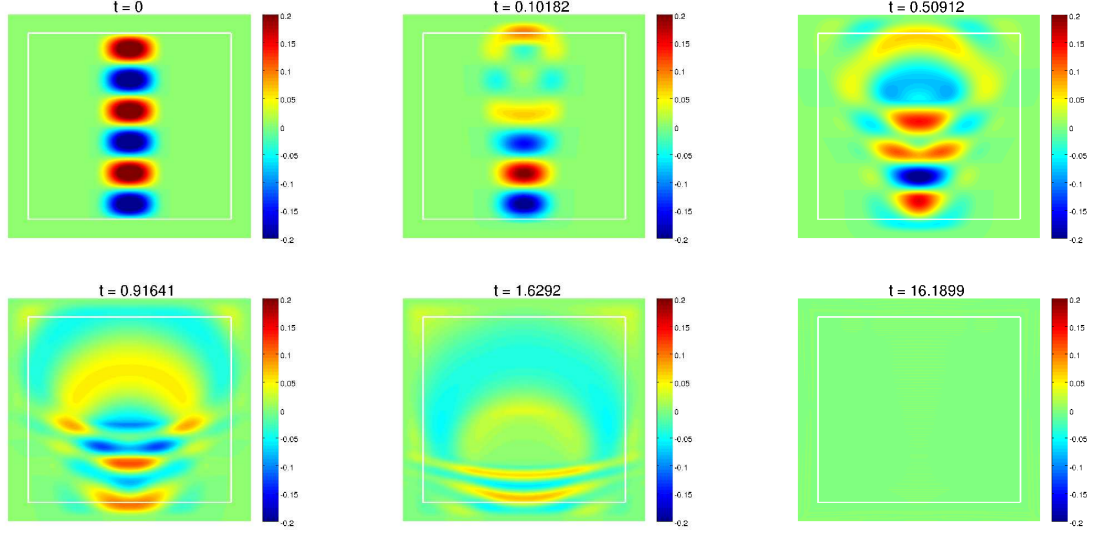


Figure 5: Heterogeneous medium in 2D: snapshots of the numerical solution are shown at different times in $\Omega = [-1, 1]^2$, surrounded by a PML of width $L = 0.2$.

5.3 Point source in 3D

Finally, we consider the wave equation (2.1) in three space dimensions with zero initial conditions and the same point source f as in (5.1). The grid spacing is uniform in x_1 , x_2 and x_3 with $\Delta x = 0.006$. In Figure 6, we display snapshots of the numerical solutions at different times in $\Omega = [-0.5, 0.5]^2$, surrounded by a PML of width $L = 0.1$. We observe how the spherical wave propagates outward essentially without spurious reflection from the PML. By time $t = 1$ the wave has essentially left the computational domain. Again we observe no instabilities in the numerical solution even at much later times.

6 Concluding remarks

We have presented a PML formulation for the wave equation in its standard second-order form. It distinguishes itself from known formulations by its simplicity and the small

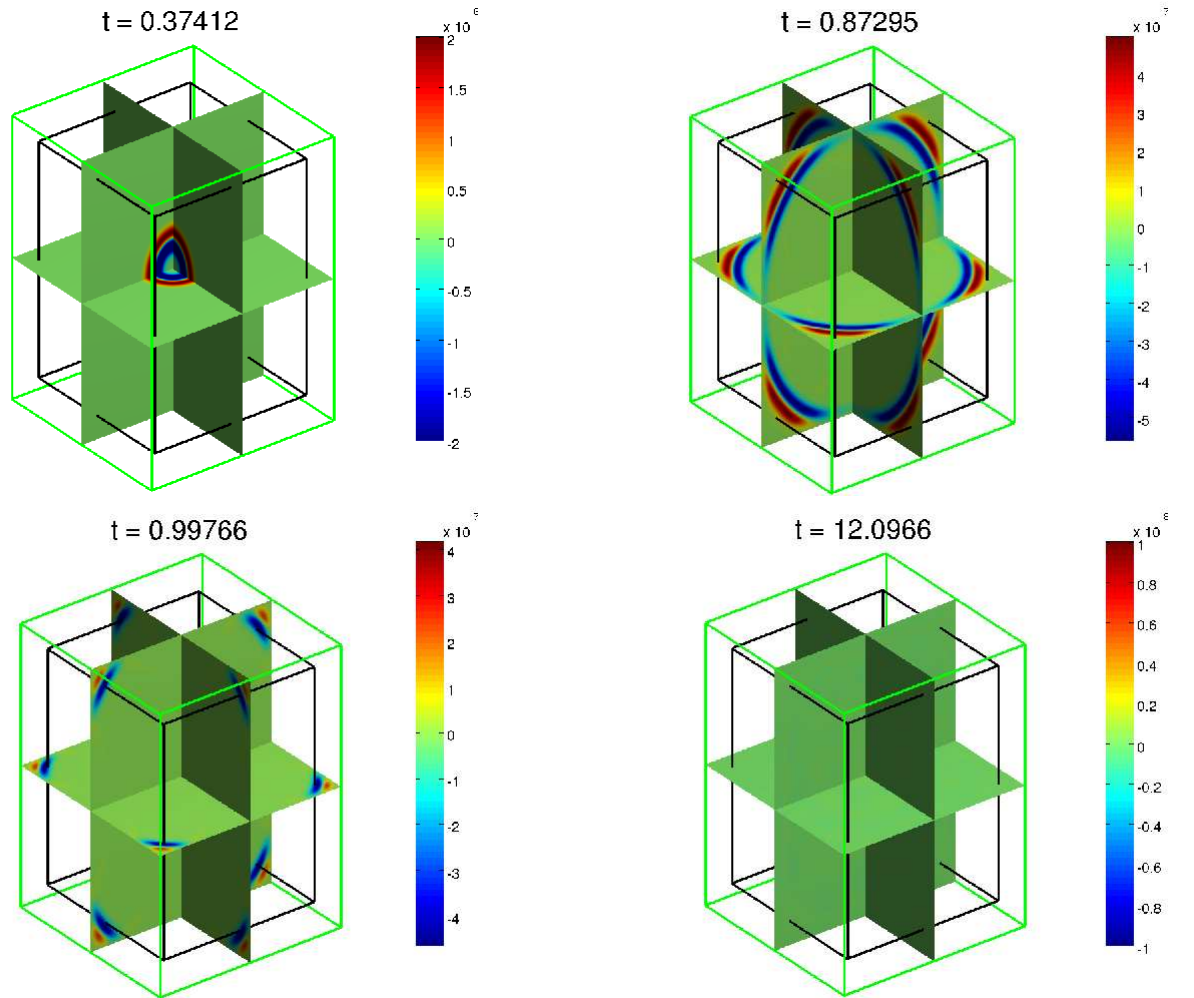


Figure 6: Point source in 3D: snapshots of the numerical solution are shown at different times in $\Omega = [-0.5, 0.5]^3$, surrounded by a PML of width $L = 0.1$.

number of auxiliary variables needed inside the absorbing layer. We have proved that the continuous Cauchy problem with the unbounded PML is stable and well-posed. Our numerical results in two and in three space dimensions with standard finite differences illustrate the accuracy, versatility and long-time stability of our PML formulation. Because it involves no high space or time derivatives, our PML formulation easily fits continuous or discontinuous Galerkin formulation for use with finite element methods [10, 13]. It also immediately generalizes to Maxwell's equations in second-order form. Current work involves the extension to second-order wave equations in complex elastic and poro-elastic media, and will be reported elsewhere in the near future.

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